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A wave-optical toolbox for multiple CRL transfocators

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Abstract. Modern synchrotron radiation sources are usually equipped with state-of-the-art focusing setups. In the last decade, modular arrays of compound refractive lenses, the so called transfocators, have emerged as adjustable focusing optics elements. Several arrays of more than one hundred lenses are distributed in the x-ray beam path to obtain optimal focusing; however, fully wave-optical simulations of such set-ups are still missing.

We present a simple toolbox of distributed computer codes to numerically propagate an x-ray beam through a sequence of transfocators, illuminated by a point-source and a partially coherent extended source.

1. Introduction

X-ray focusing using compound refractive lenses (CRLs) [1] has proven to be very effective over the last two decades. It is now some years, since interchangeable arrays of lenses, so called transfocators, have allowed for easy and fast adaptation of the number of lenses to match focal length and photon energy [2, 3]. An increasing number of experiments makes use of combined optics, i.e. two transfocators placed large distances apart. For individual lenses are placed several millimetres apart, a transfocator should not be treated as a “thin lens”. This makes analytical treatments difficult.

We are developing a wave-optical simulation code that propagates a point-source or a partially coherent source through a sequence of transfocators that can be placed several metres apart. Lens stacking errors (misalignment, rough surfaces of wrong shape etc.) are foreseen for future versions.

2. Theory

Wave-optical approaches often need many approximations to solve numerically Maxwell’s equations. In the following, we will assume illumination by a monochromatic point-source of in-vacuum wavelength λ ; individual lenses are treated as “thin lenses” described by an optical transfer function τ . Propagation from lens to lens is carried out in Fourier space [4]; free space propagation between different transfocators is carried out solving Fresnel-Kirchhoff’s diffraction integral. A partially coherent source is modelled using a stochastic optical fields method [5, 6]. So far, all simulations are done in “one plus one dimension”.

2.1. Individual lens

If one treats a single lens as a “thin object”, the lens can be modelled by an optical transfer function $\tau(y)$, y being one lateral coordinate:

$$\tau(y) = \exp(-i\pi y^2 / \lambda f), \quad (1)$$

for a lens of focal length f ; the lens is assumed to be of parabolic shape. Such lenses are widely used and appear to be good approximations of the ideal Cartesian oval [7]. The phase factor (1) multiplies the incoming, complex-valued illumination field. Absorption effects can also be included with an additional real-valued exponential term.

2.2. Case of one transfocator

An array of individual lenses is modelled by Fourier propagation between individual lenses and multiplication of the corresponding phase factors at each lens plane. The outgoing field ψ_n is then propagated to the preceding lens plane by a distance Δx using the Fourier propagator [4]

$$\psi_{n+1} \propto \exp(i y^2 / 2k \Delta x) \text{FFT} [\exp(i y^2 / 2k \Delta x) \psi_n]. \quad (2)$$

For the fast Fourier transform to work properly, the computational grid has to be chosen adequately. Depending on wavelength and geometrical parameters, individual lenses can be simulated in less than one second on “typical” single-core CPUs.

2.3. Case of several transfocators

The outgoing wave-field ψ_m of one transfocator can be propagated to the next by solving the Fresnel-Kirchhoff diffraction integral

$$\psi_{m+1} \propto \sum_y \psi_m(y) \exp(i \vec{k} \cdot \vec{r}) / r.$$

Since the phase term $\exp(ikr)$ oscillates strongly, a Taylor expansion of the local distance vector $r = \sqrt{\Delta x^2 + \Delta y^2}$ is necessary to reduce complexity and numerical errors. Using the Fourier propagator (2), the number of points on both planes is of the order of 10^6 , thus requiring about 10^{12} calculations. For this to work efficiently, we make use of current CUDA [8] graphics cards that allow for massive parallelism (more than 10^3 calculations in parallel). This reduces the heavy computational overhead implied in fully wave-optical free-space propagation, which would take otherwise many hours, to several minutes.

2.4. Partial coherence

Propagating N individual point-sources from a virtual extended source results in a set of *basic fields* u_n in a given region of interest. A stochastic superposition

$$U = \sum_n w_n c_n u_n$$

represents a single *realisation* of the fluctuating wave-field (due to missing correlation between points in the source) [5, 6]. The real coefficients w_n describe the source’s envelope, the random complex coefficients c_n the instantaneous strength and phase relation of individual point sources. We then define the mutual intensity $\Gamma_{1,2}$,

$$\Gamma_{1,2} = \langle U(1)^* U(2) \rangle, \quad (3)$$

as the ensemble average of such realisations with different random coefficients c_n . Since the source envelope w_n appears only in the averaging, pre-calculated u_n can be re-used independently of source size and source profile.

From (3), we can easily extract both partially coherent intensity $I(1) = \Gamma(1, 1)$ and degree of coherence $\gamma(1, 2) = \Gamma(1, 2) / \sqrt{\Gamma(1, 1)\Gamma(2, 2)}$.

The source size that enters in the envelope coefficients w_n can either be measured with an interferometer or simulated, e.g. with SRW (Synchrotron Radiation Workshop) [9]. The source's finite emittance can be included with correlated random coefficients c_n ; this is currently under investigation.

3. Programmes

3.1. General layout

Our computational toolbox consists of three individual programmes that communicate with each other by sending hypertext transfer protocol (HTTP) commands. This has several advantages:

- The CUDA code can run on a remote machine compared to the single transfocator code; the machines do not even need a common file system.
- Using proxy servers, load balancing could be achieved transparently for the simulation programmes.
- Scripts and third-party software can control simulation runs and access data using standardised HTTP commands.
- A web-based graphical user interface is accessible from virtually *everywhere*, with optional encryption using an SSL proxy.

3.2. Case of one transfocator

The tool *XSTS* (X-ray Single Transfocator Simulation) propagates an illuminating source (either a point-source or an incoming complex-valued field) through an array of compound refractive lenses. The user can access the complex valued field and simple plots of intensity and phase after each lens from the web GUI (see below). As a typical example, the ID 11 transfocator [10] has been simulated; for a photon energy of 29.6 keV, a point-source at 92.5 m is focused by 128 Be lenses (focal distance 1.8483 m) to a spot of 760 nm (FWHM).

3.3. Case of several transfocators

The tool *XMTS* (X-ray Multiple Transfocator Simulation) carries out the free-space propagation from one transfocator to the next; the user can easily access the intensity and phase information (data plus plot) on both planes.

These two tools are not considered stable and are thus not yet released publicly.

3.4. Partial coherence

The stochastic superposition simulating a (spatially) partially coherent source is carried out by a third programme (see online material of [5]). This code reads pre-calculated basic fields u_n and outputs the ensemble averaged mutual intensity and degree of coherence.

4. Summary and Outlook

We are developing a wave-optical toolbox to simulate sequences of transfocators, each consisting of multiple compound refractive lenses. The package will be released as soon as all the individual modules are considered to be stable and reliable. An α -version of the code can be obtained upon request from the corresponding author (MO).

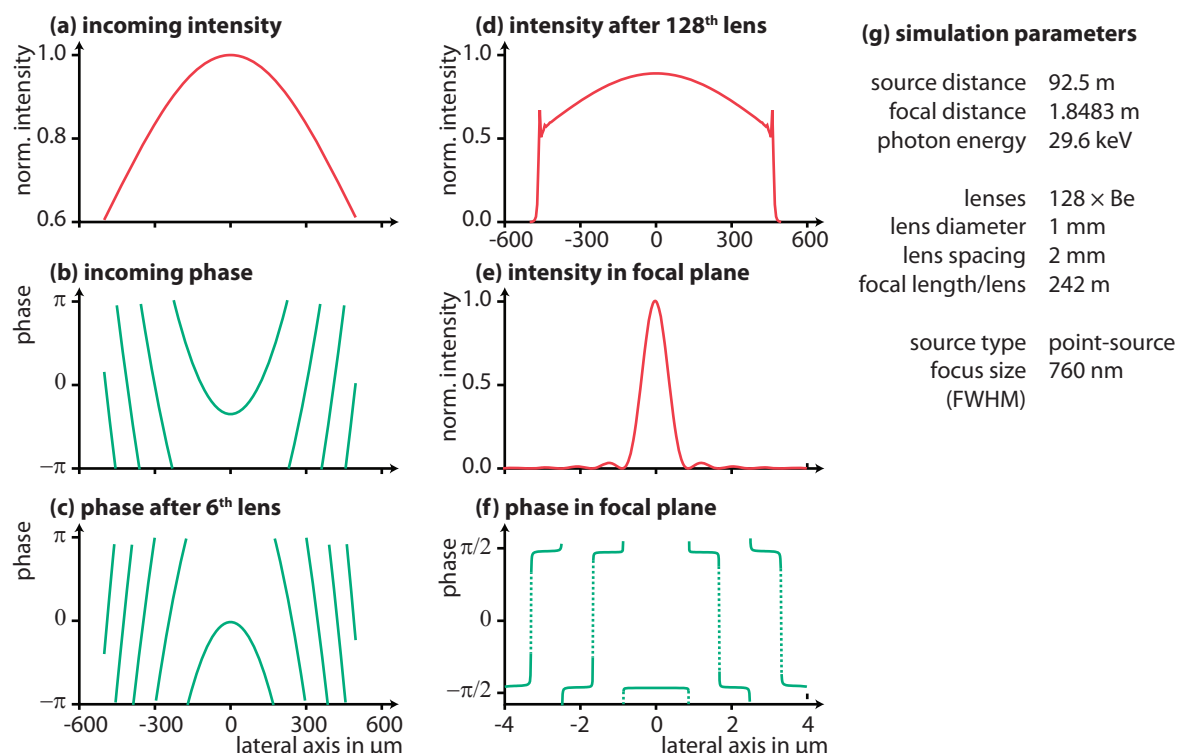


Figure 1. Simulated intensity and phase evolution inside a typical translocator (a-d) and in the focal plane (e,f); relevant parameters are shown in (g) and correspond to the ID11 beamline at the ESRF [10].

For future versions, several generalisations are under development, most notably misalignments of lenses (tip/tilt, misplacements), surface errors, and polychromatic sources which generate chromatic aberrations.

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